



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 6, 2026 – 02:20 pm BST

PDB ID : 9RTQ / pdb_00009rtq
Title : Crystal structure of BRAF:MEK1 complex with symmetric dimer interface bound to AMPPNP
Authors : Kondo, Y.; Notbohm, J.; Camacho, I.N.; Nagy-Davidescu, G.; Mason, T.; Muhle, J.; Standfuss, J.; Perica, T.
Deposited on : 2025-07-03
Resolution : 2.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

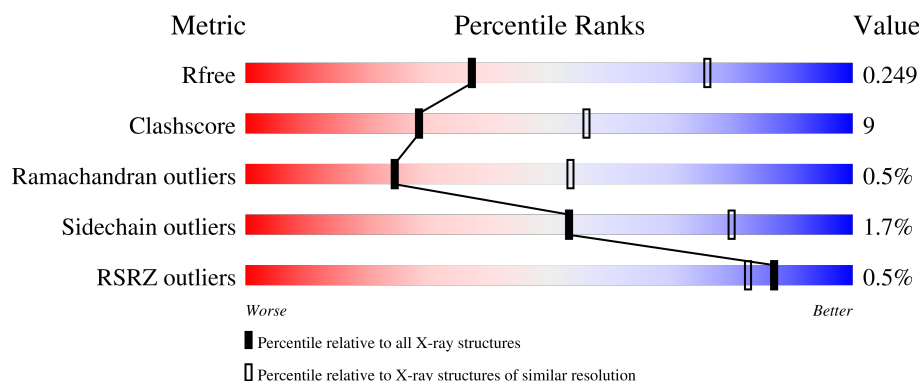
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	282	
1	C	282	
1	F	282	
1	G	282	

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Mol	Chain	Length	Quality of chain
2	A	333	% 66% 20% 14%
2	D	333	% 65% 21% • 13%
2	E	333	% 62% 23% • 14%
2	H	333	% 64% 21% 15%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17739 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	262	Total	C	N	O	S	0	0	0
			2105	1336	373	383	13			
1	C	261	Total	C	N	O	S	0	1	0
			2107	1340	373	381	13			
1	F	263	Total	C	N	O	S	0	2	0
			2129	1353	377	386	13			
1	G	259	Total	C	N	O	S	0	1	0
			2090	1329	370	378	13			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	442	SER	-	expression tag	UNP P15056
B	443	ASN	-	expression tag	UNP P15056
B	444	ALA	-	expression tag	UNP P15056
B	543	ALA	ILE	engineered mutation	UNP P15056
B	544	SER	ILE	engineered mutation	UNP P15056
B	551	LYS	ILE	engineered mutation	UNP P15056
B	562	ARG	GLN	engineered mutation	UNP P15056
B	588	ASN	LEU	engineered mutation	UNP P15056
B	600	GLU	VAL	conflict	UNP P15056
B	630	SER	LYS	engineered mutation	UNP P15056
B	688	ARG	ALA	engineered mutation	UNP P15056
B	706	SER	LEU	engineered mutation	UNP P15056
B	709	ARG	GLN	conflict	UNP P15056
B	713	GLU	SER	engineered mutation	UNP P15056
B	716	GLU	LEU	engineered mutation	UNP P15056
B	720	GLU	SER	engineered mutation	UNP P15056
B	722	SER	-	expression tag	UNP P15056
B	723	GLY	-	expression tag	UNP P15056
C	442	SER	-	expression tag	UNP P15056
C	443	ASN	-	expression tag	UNP P15056
C	444	ALA	-	expression tag	UNP P15056

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Chain	Residue	Modelled	Actual	Comment	Reference
C	543	ALA	ILE	engineered mutation	UNP P15056
C	544	SER	ILE	engineered mutation	UNP P15056
C	551	LYS	ILE	engineered mutation	UNP P15056
C	562	ARG	GLN	engineered mutation	UNP P15056
C	588	ASN	LEU	engineered mutation	UNP P15056
C	600	GLU	VAL	conflict	UNP P15056
C	630	SER	LYS	engineered mutation	UNP P15056
C	688	ARG	ALA	engineered mutation	UNP P15056
C	706	SER	LEU	engineered mutation	UNP P15056
C	709	ARG	GLN	conflict	UNP P15056
C	713	GLU	SER	engineered mutation	UNP P15056
C	716	GLU	LEU	engineered mutation	UNP P15056
C	720	GLU	SER	engineered mutation	UNP P15056
C	722	SER	-	expression tag	UNP P15056
C	723	GLY	-	expression tag	UNP P15056
F	442	SER	-	expression tag	UNP P15056
F	443	ASN	-	expression tag	UNP P15056
F	444	ALA	-	expression tag	UNP P15056
F	543	ALA	ILE	engineered mutation	UNP P15056
F	544	SER	ILE	engineered mutation	UNP P15056
F	551	LYS	ILE	engineered mutation	UNP P15056
F	562	ARG	GLN	engineered mutation	UNP P15056
F	588	ASN	LEU	engineered mutation	UNP P15056
F	600	GLU	VAL	conflict	UNP P15056
F	630	SER	LYS	engineered mutation	UNP P15056
F	688	ARG	ALA	engineered mutation	UNP P15056
F	706	SER	LEU	engineered mutation	UNP P15056
F	709	ARG	GLN	conflict	UNP P15056
F	713	GLU	SER	engineered mutation	UNP P15056
F	716	GLU	LEU	engineered mutation	UNP P15056
F	720	GLU	SER	engineered mutation	UNP P15056
F	722	SER	-	expression tag	UNP P15056
F	723	GLY	-	expression tag	UNP P15056
G	442	SER	-	expression tag	UNP P15056
G	443	ASN	-	expression tag	UNP P15056
G	444	ALA	-	expression tag	UNP P15056
G	543	ALA	ILE	engineered mutation	UNP P15056
G	544	SER	ILE	engineered mutation	UNP P15056
G	551	LYS	ILE	engineered mutation	UNP P15056
G	562	ARG	GLN	engineered mutation	UNP P15056
G	588	ASN	LEU	engineered mutation	UNP P15056
G	600	GLU	VAL	conflict	UNP P15056

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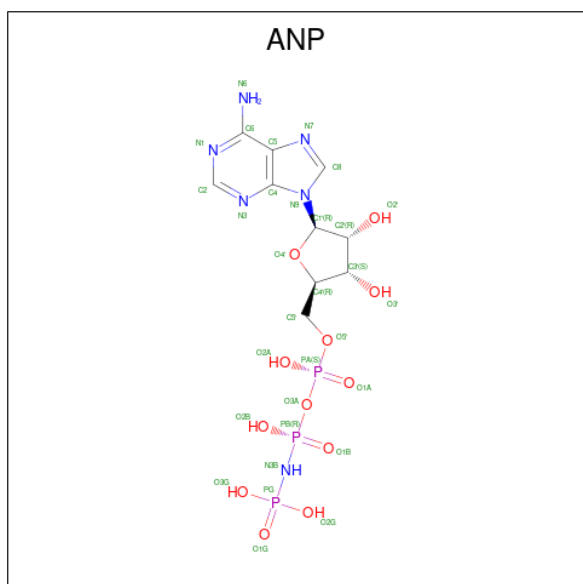
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Chain	Residue	Modelled	Actual	Comment	Reference
G	630	SER	LYS	engineered mutation	UNP P15056
G	688	ARG	ALA	engineered mutation	UNP P15056
G	706	SER	LEU	engineered mutation	UNP P15056
G	709	ARG	GLN	conflict	UNP P15056
G	713	GLU	SER	engineered mutation	UNP P15056
G	716	GLU	LEU	engineered mutation	UNP P15056
G	720	GLU	SER	engineered mutation	UNP P15056
G	722	SER	-	expression tag	UNP P15056
G	723	GLY	-	expression tag	UNP P15056

- Molecule 2 is a protein called Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	290	Total	C	N	O	S	0	1	0
			2273	1454	383	420	16			
2	A	288	Total	C	N	O	S	0	0	0
			2253	1440	381	416	16			
2	H	284	Total	C	N	O	S	0	0	0
			2224	1422	376	410	16			
2	E	286	Total	C	N	O	S	0	0	0
			2236	1431	378	411	16			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

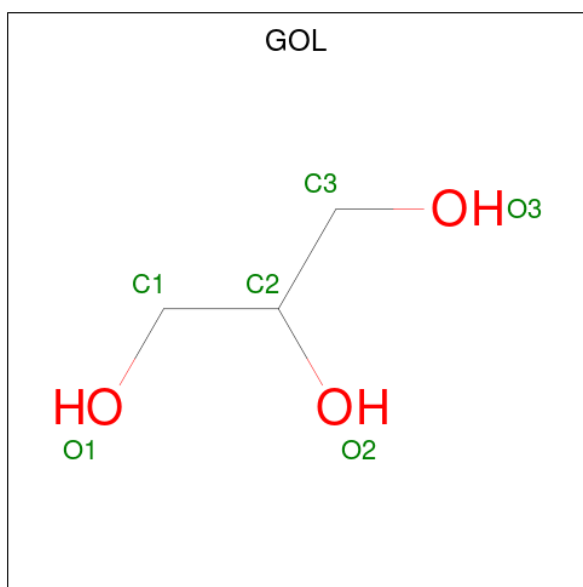


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	2	Total	Ca	0	0
			2	2		
4	A	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		
4	G	1	Total	Ca	0	0
			1	1		
4	H	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

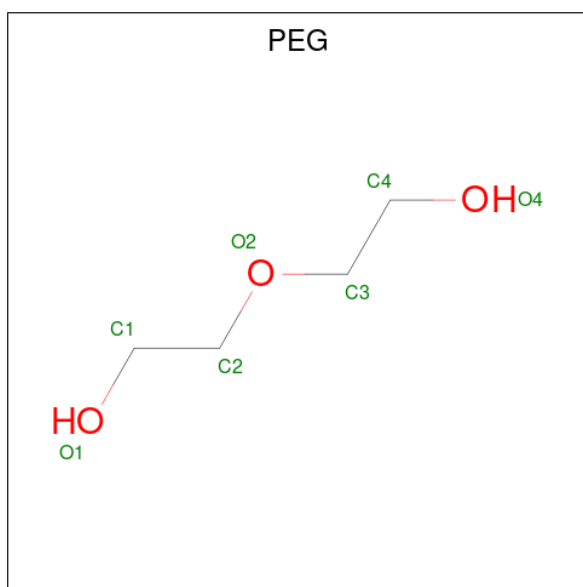


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		
6	H	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			7	4	3		
7	H	1	Total	C	O	0	0
			7	4	3		

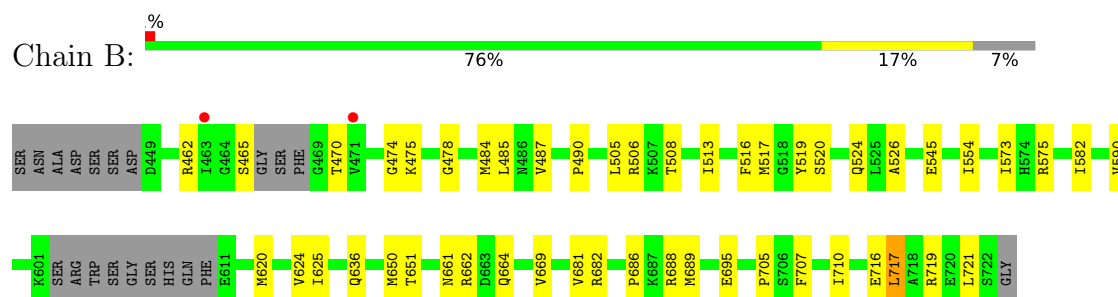
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	5	Total	O	0	0
			5	5		
8	C	2	Total	O	0	0
			2	2		
8	D	3	Total	O	0	0
			3	3		
8	A	4	Total	O	0	0
			4	4		
8	F	6	Total	O	0	0
			6	6		
8	G	2	Total	O	0	0
			2	2		
8	H	3	Total	O	0	0
			3	3		
8	E	5	Total	O	0	0
			5	5		

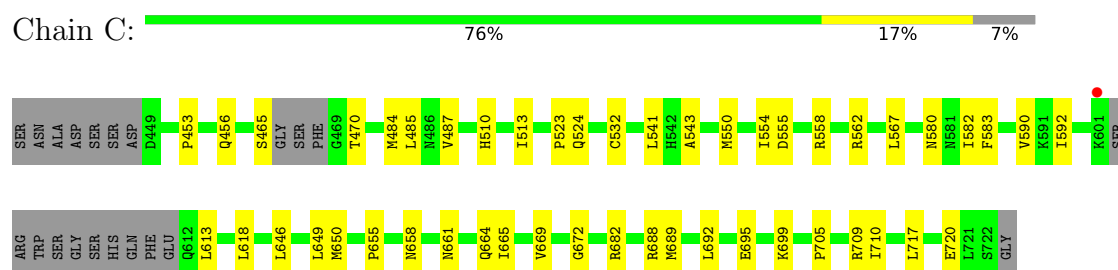
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

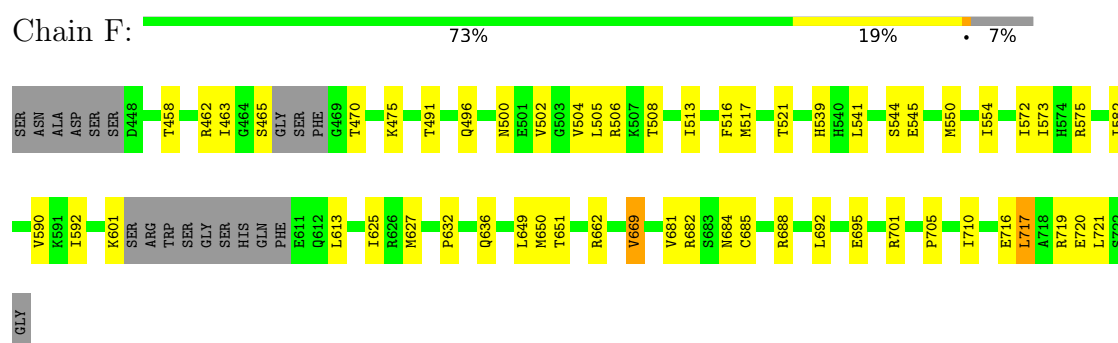
- Molecule 1: Serine/threonine-protein kinase B-raf



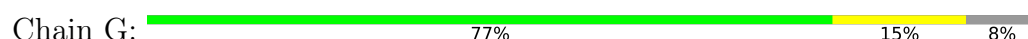
- Molecule 1: Serine/threonine-protein kinase B-raf



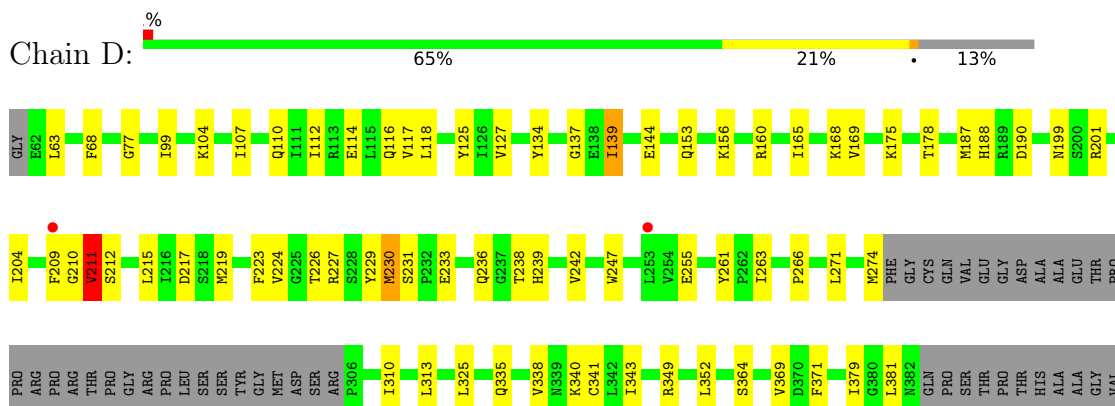
- Molecule 1: Serine/threonine-protein kinase B-raf



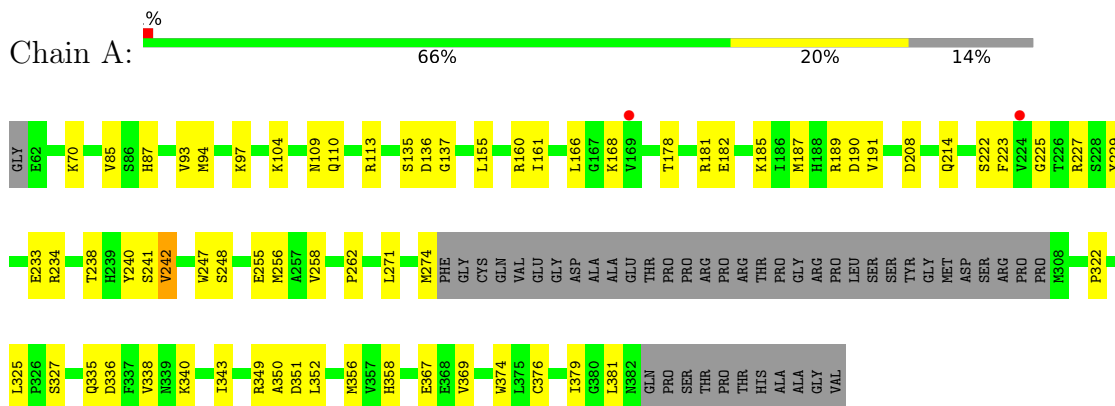
- Molecule 1: Serine/threonine-protein kinase B-raf



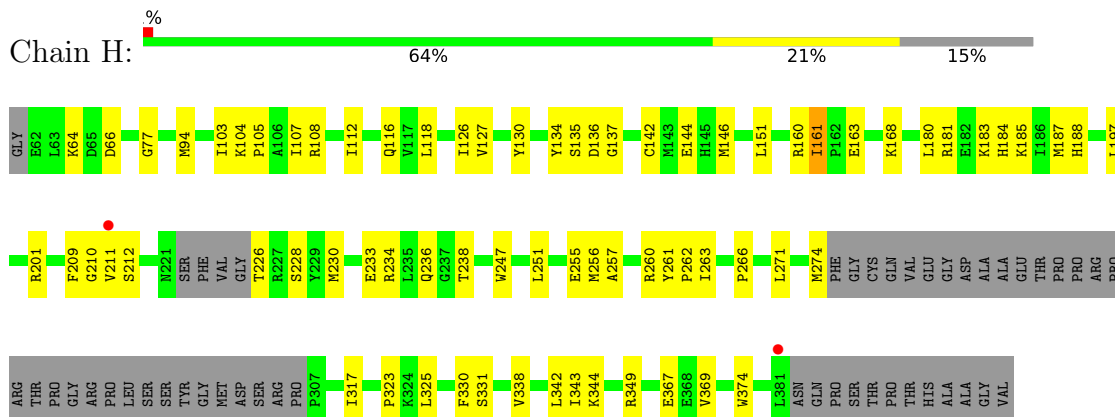
- Molecule 2: Dual specificity mitogen-activated protein kinase kinase 1



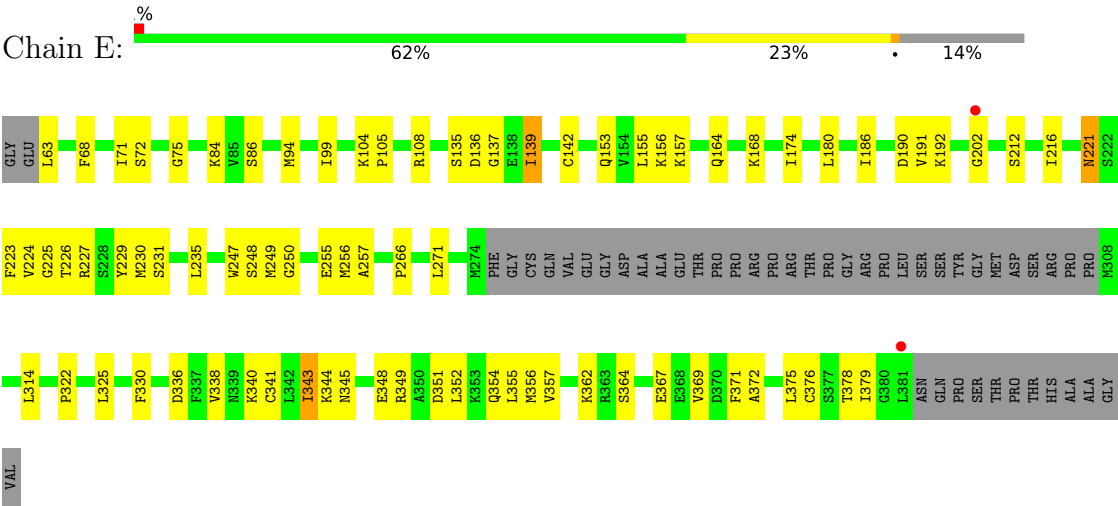
- Molecule 2: Dual specificity mitogen-activated protein kinase kinase 1



- Molecule 2: Dual specificity mitogen-activated protein kinase kinase 1



- Molecule 2: Dual specificity mitogen-activated protein kinase kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.63Å 163.87Å 201.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.91 48.06 – 2.91	Depositor EDS
% Data completeness (in resolution range)	78.9 (48.06-2.91) 78.8 (48.06-2.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.205 , 0.250 0.206 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 89.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17739	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5781e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CA, CL, GOL, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.17	0/2147	0.35	0/2891
1	C	0.16	0/2150	0.33	0/2895
1	F	0.18	0/2178	0.35	0/2932
1	G	0.14	0/2133	0.30	0/2872
2	A	0.18	0/2298	0.39	0/3097
2	D	0.17	0/2323	0.38	0/3132
2	E	0.28	0/2281	0.47	1/3074 (0.0%)
2	H	0.16	0/2268	0.38	0/3055
All	All	0.19	0/17778	0.37	1/23948 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	343	ILE	N-CA-C	-5.12	100.52	107.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	181	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2105	0	2124	29	0
1	C	2107	0	2126	35	0
1	F	2129	0	2150	33	0
1	G	2090	0	2107	28	0
2	A	2253	0	2280	42	0
2	D	2273	0	2301	47	0
2	E	2236	0	2268	61	0
2	H	2224	0	2255	45	0
3	A	31	0	13	0	0
3	B	31	0	13	1	0
3	C	31	0	13	3	0
3	D	31	0	13	2	0
3	E	31	0	13	1	0
3	F	31	0	13	0	0
3	G	31	0	13	2	0
3	H	31	0	13	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	F	6	0	8	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
7	D	7	0	10	0	0
7	H	7	0	10	1	0
8	A	4	0	0	0	0
8	B	5	0	0	0	0
8	C	2	0	0	0	0
8	D	3	0	0	1	0
8	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	6	0	0	0	0
8	G	2	0	0	0	0
8	H	3	0	0	0	0
All	All	17739	0	17759	311	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 311 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:247:TRP:HE3	2:E:349:ARG:NH2	1.67	0.93
2:E:376:CYS:HA	2:E:379:ILE:HG12	1.53	0.89
2:A:227:ARG:NH1	2:A:229:TYR:OH	2.11	0.82
1:B:462:ARG:NH1	1:B:465:SER:OG	2.13	0.81
1:G:661:ASN:HD21	2:H:230:MET:HE2	1.46	0.81

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	256/282 (91%)	249 (97%)	7 (3%)	0	100	100
1	C	256/282 (91%)	250 (98%)	5 (2%)	1 (0%)	30	58
1	F	259/282 (92%)	250 (96%)	9 (4%)	0	100	100
1	G	254/282 (90%)	246 (97%)	6 (2%)	2 (1%)	16	43
2	A	284/333 (85%)	273 (96%)	10 (4%)	1 (0%)	30	58
2	D	287/333 (86%)	278 (97%)	7 (2%)	2 (1%)	18	46
2	E	282/333 (85%)	273 (97%)	8 (3%)	1 (0%)	30	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	278/333 (84%)	270 (97%)	5 (2%)	3 (1%)	11	35
All	All	2156/2460 (88%)	2089 (97%)	57 (3%)	10 (0%)	24	53

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	211	VAL
2	A	190	ASP
2	H	136	ASP
2	H	184	HIS
2	H	211	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	231/247 (94%)	227 (98%)	4 (2%)	53	80
1	C	231/247 (94%)	230 (100%)	1 (0%)	84	94
1	F	234/247 (95%)	226 (97%)	8 (3%)	32	65
1	G	229/247 (93%)	229 (100%)	0	100	100
2	A	250/285 (88%)	246 (98%)	4 (2%)	55	81
2	D	253/285 (89%)	247 (98%)	6 (2%)	43	73
2	E	248/285 (87%)	243 (98%)	5 (2%)	48	77
2	H	247/285 (87%)	242 (98%)	5 (2%)	48	77
All	All	1923/2128 (90%)	1890 (98%)	33 (2%)	53	80

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	139	ILE
2	E	221	ASN
2	E	230	MET
2	A	135	SER

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Mol	Chain	Res	Type
2	A	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	221	ASN
2	E	221	ASN
2	E	354	GLN
2	E	145	HIS
1	F	612	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ANP	A	901	4	32,33,33	0.99	5 (15%)	44,52,52	0.81	2 (4%)
5	GOL	F	903	-	5,5,5	0.98	0	5,5,5	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	B	901	4	32,33,33	0.95	4 (12%)	44,52,52	1.00	3 (6%)
7	PEG	H	904	-	6,6,6	0.13	0	5,5,5	0.07	0
5	GOL	B	903	-	5,5,5	0.95	0	5,5,5	0.89	0
3	ANP	E	901	4	32,33,33	0.97	4 (12%)	44,52,52	0.94	4 (9%)
7	PEG	D	904	-	6,6,6	0.15	0	5,5,5	0.05	0
3	ANP	F	901	4	32,33,33	0.95	4 (12%)	44,52,52	0.95	2 (4%)
3	ANP	H	901	4	32,33,33	0.95	4 (12%)	44,52,52	0.80	1 (2%)
3	ANP	D	901	4	32,33,33	0.98	5 (15%)	44,52,52	0.81	1 (2%)
3	ANP	G	901	4	32,33,33	0.94	4 (12%)	44,52,52	0.79	2 (4%)
3	ANP	C	901	4	32,33,33	0.95	4 (12%)	44,52,52	0.77	1 (2%)
5	GOL	C	903	-	5,5,5	0.97	0	5,5,5	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	901	4	-	6/18/38/38	0/3/3/3
5	GOL	F	903	-	-	0/4/4/4	-
3	ANP	B	901	4	-	8/18/38/38	0/3/3/3
7	PEG	H	904	-	-	4/4/4/4	-
5	GOL	B	903	-	-	4/4/4/4	-
3	ANP	E	901	4	-	7/18/38/38	0/3/3/3
7	PEG	D	904	-	-	0/4/4/4	-
3	ANP	F	901	4	-	7/18/38/38	0/3/3/3
3	ANP	H	901	4	-	11/18/38/38	0/3/3/3
3	ANP	D	901	4	-	4/18/38/38	0/3/3/3
3	ANP	G	901	4	-	3/18/38/38	0/3/3/3
3	ANP	C	901	4	-	3/18/38/38	0/3/3/3
5	GOL	C	903	-	-	2/4/4/4	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	901	ANP	PG-N3B	2.90	1.70	1.63
3	A	901	ANP	PG-N3B	2.84	1.70	1.63
3	C	901	ANP	PG-O1G	2.72	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	ANP	PG-N3B	2.71	1.70	1.63
3	B	901	ANP	PG-N3B	2.68	1.70	1.63

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	ANP	PB-O3A-PA	-3.48	120.35	132.62
3	H	901	ANP	PB-O3A-PA	-3.40	120.63	132.62
3	E	901	ANP	PB-O3A-PA	-3.24	121.20	132.62
3	F	901	ANP	PB-O3A-PA	-3.14	121.57	132.62
3	C	901	ANP	PB-O3A-PA	-3.10	121.68	132.62

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	901	ANP	PG-N3B-PB-O1B
3	B	901	ANP	PA-O3A-PB-O1B
3	B	901	ANP	PA-O3A-PB-O2B
3	B	901	ANP	C5'-O5'-PA-O1A
3	B	901	ANP	C5'-O5'-PA-O2A

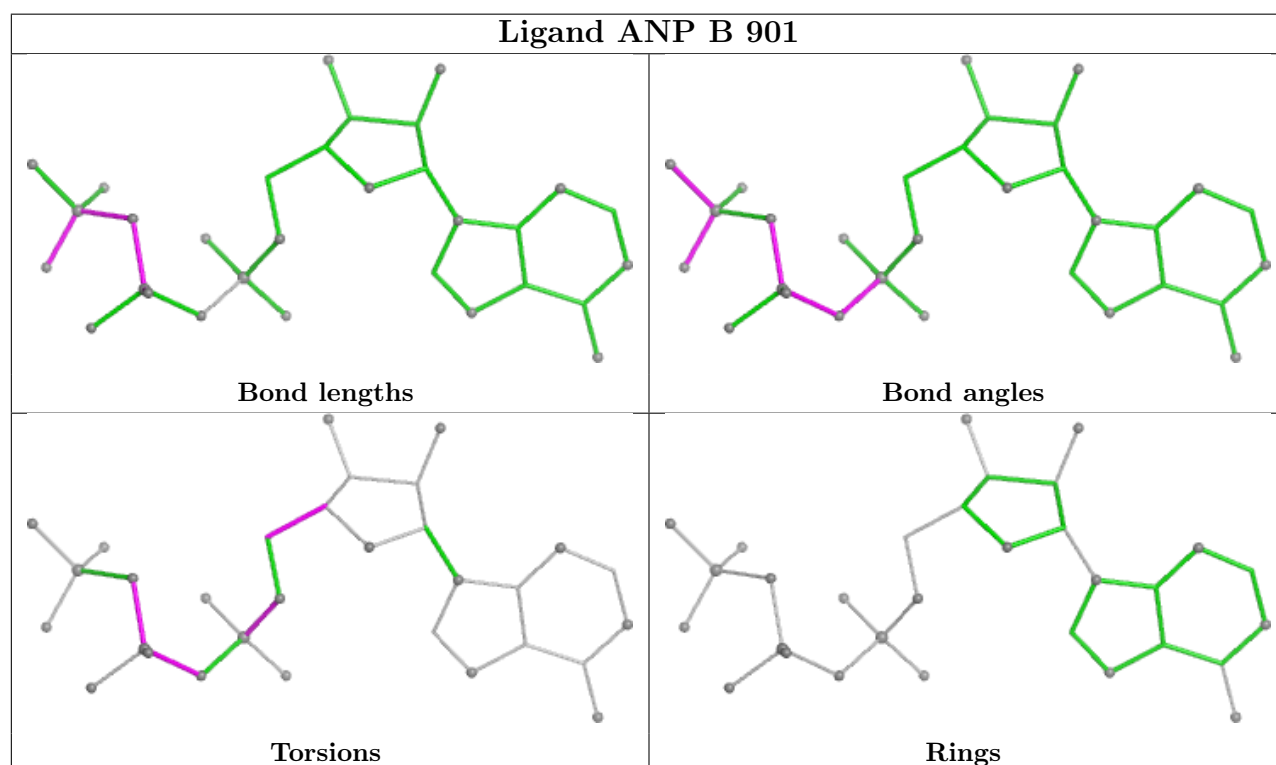
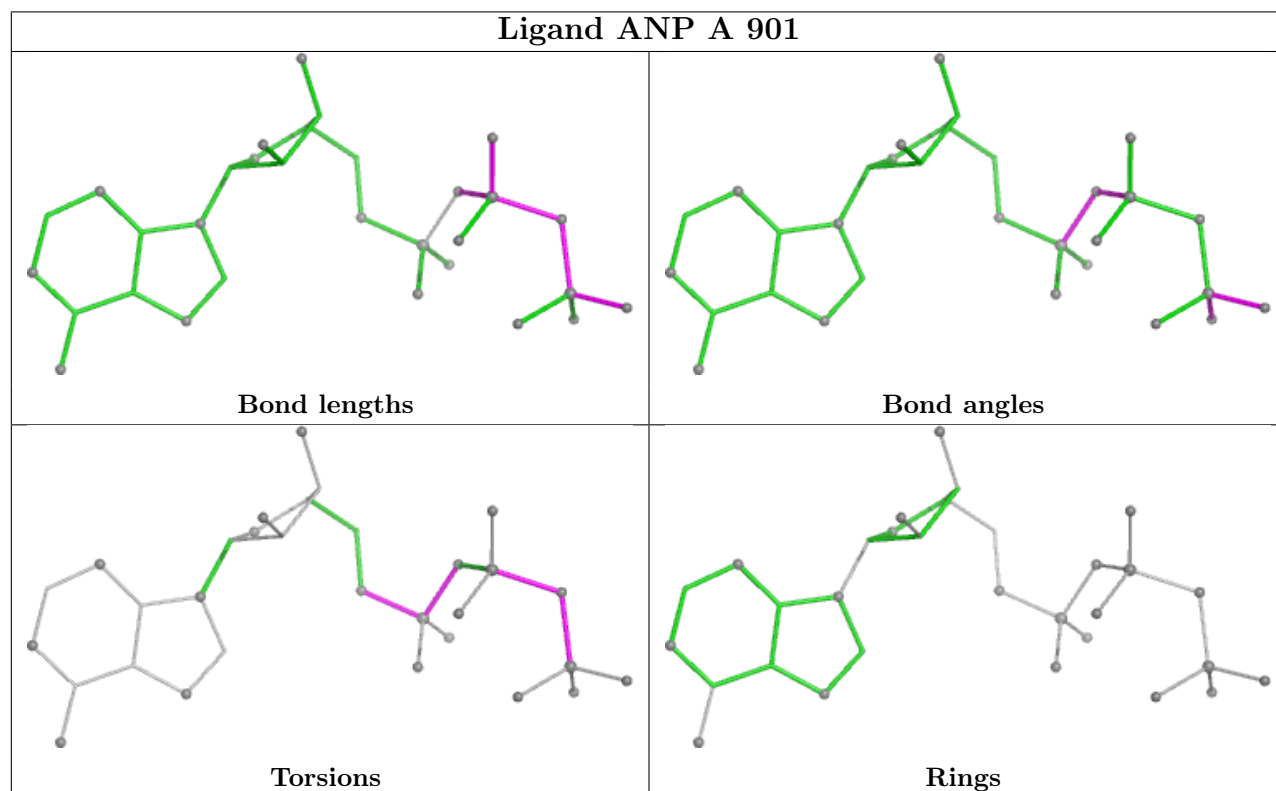
There are no ring outliers.

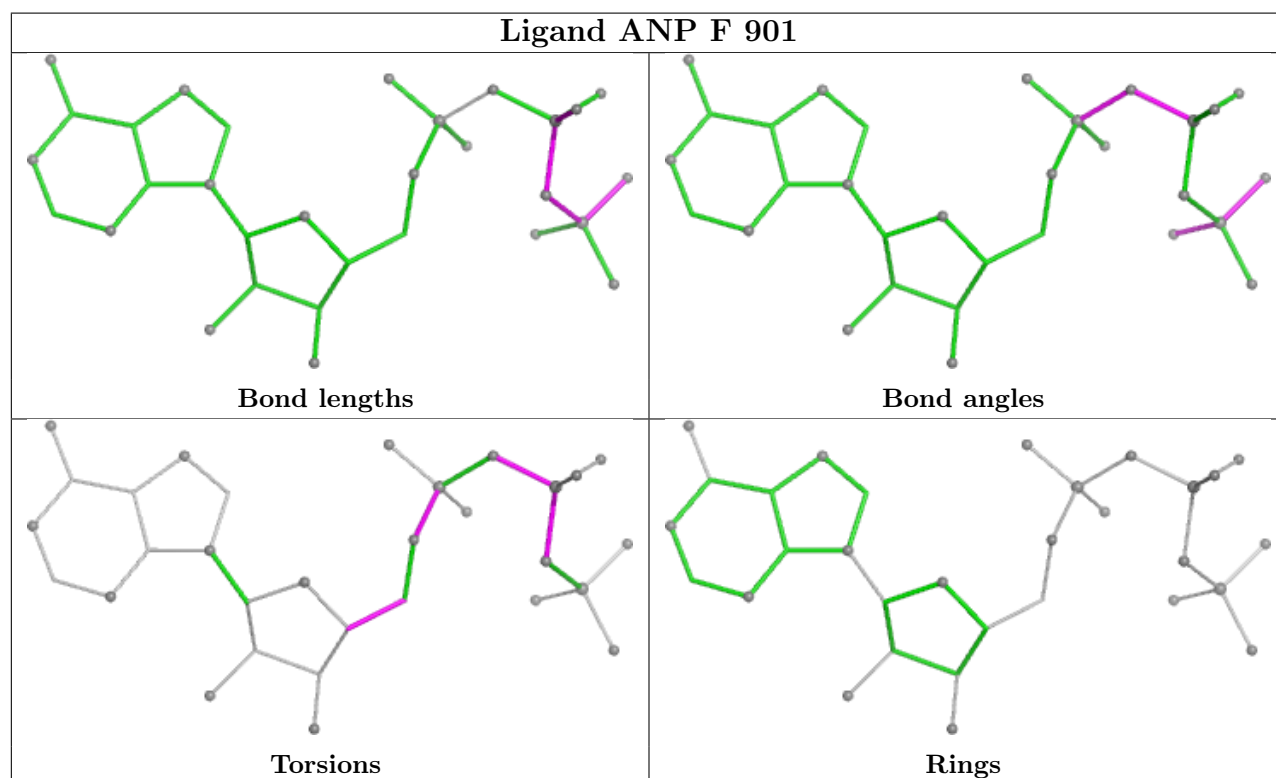
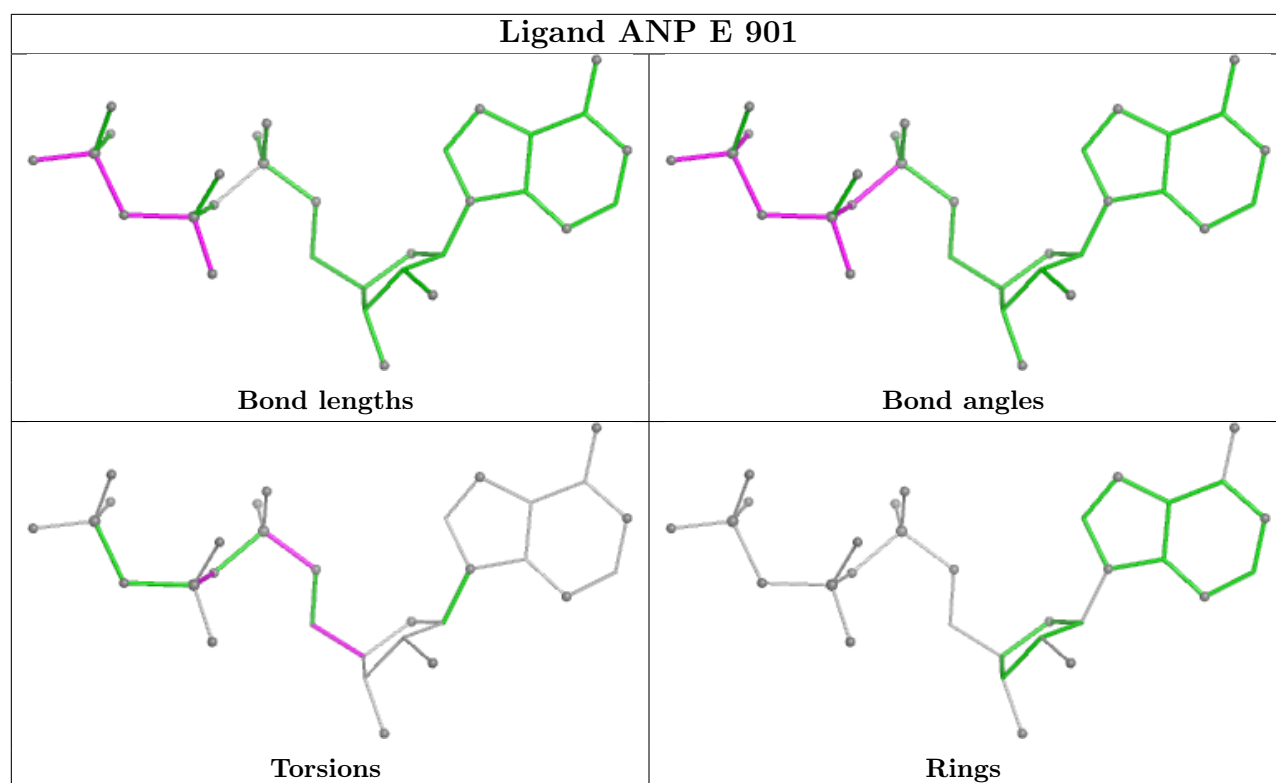
7 monomers are involved in 12 short contacts:

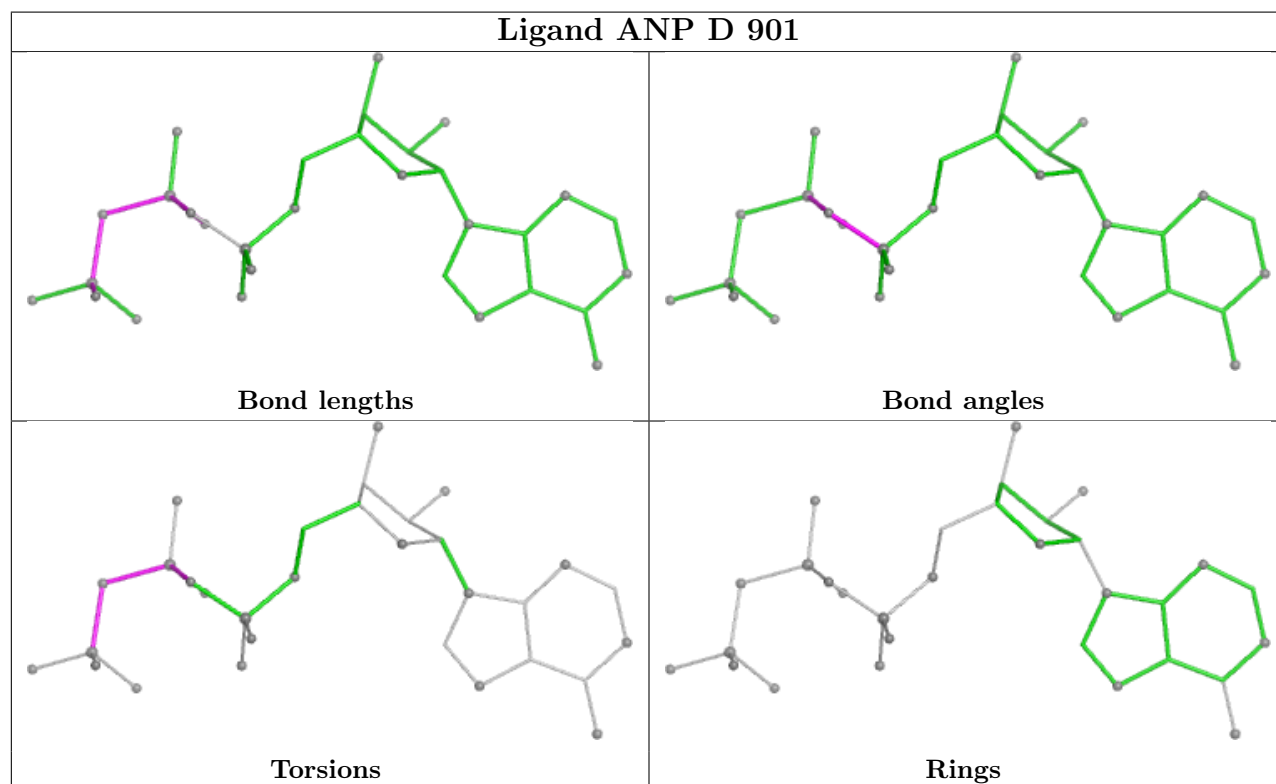
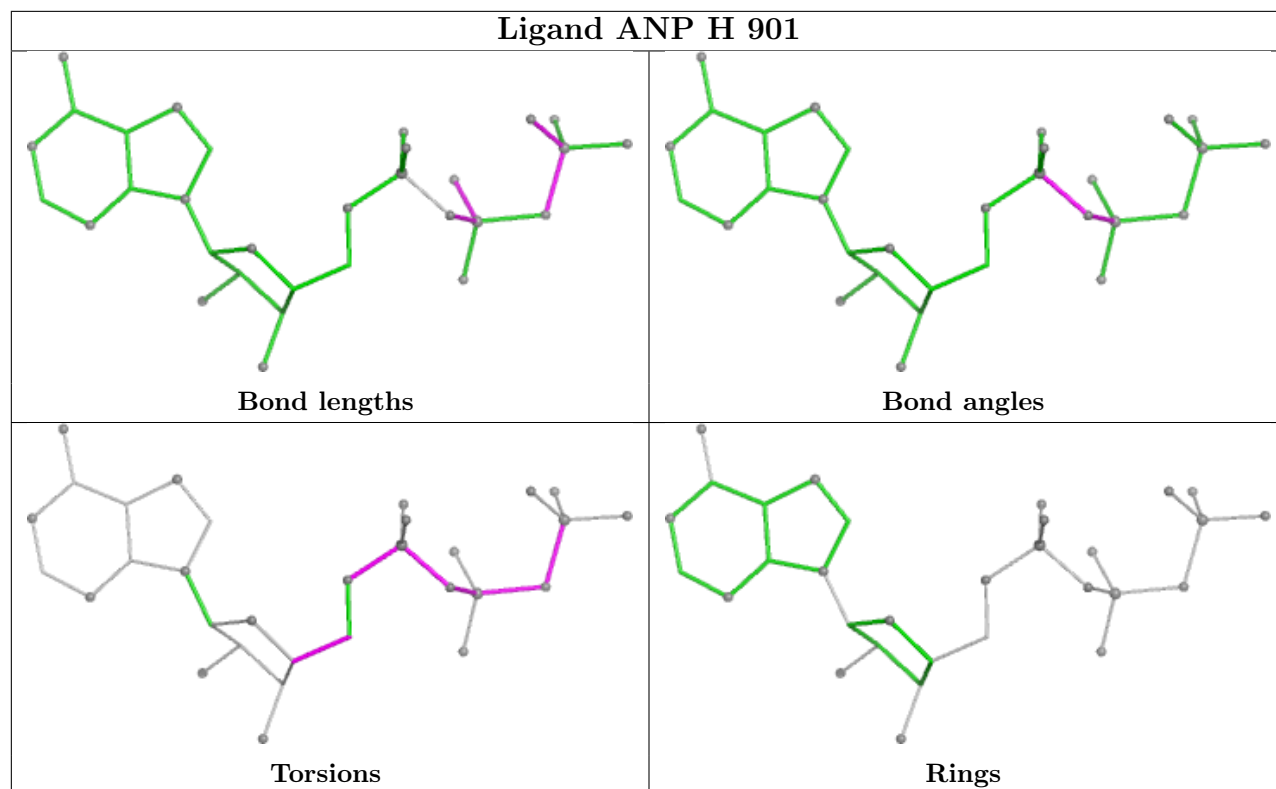
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	ANP	1	0
7	H	904	PEG	1	0
3	E	901	ANP	1	0
3	H	901	ANP	2	0
3	D	901	ANP	2	0
3	G	901	ANP	2	0
3	C	901	ANP	3	0

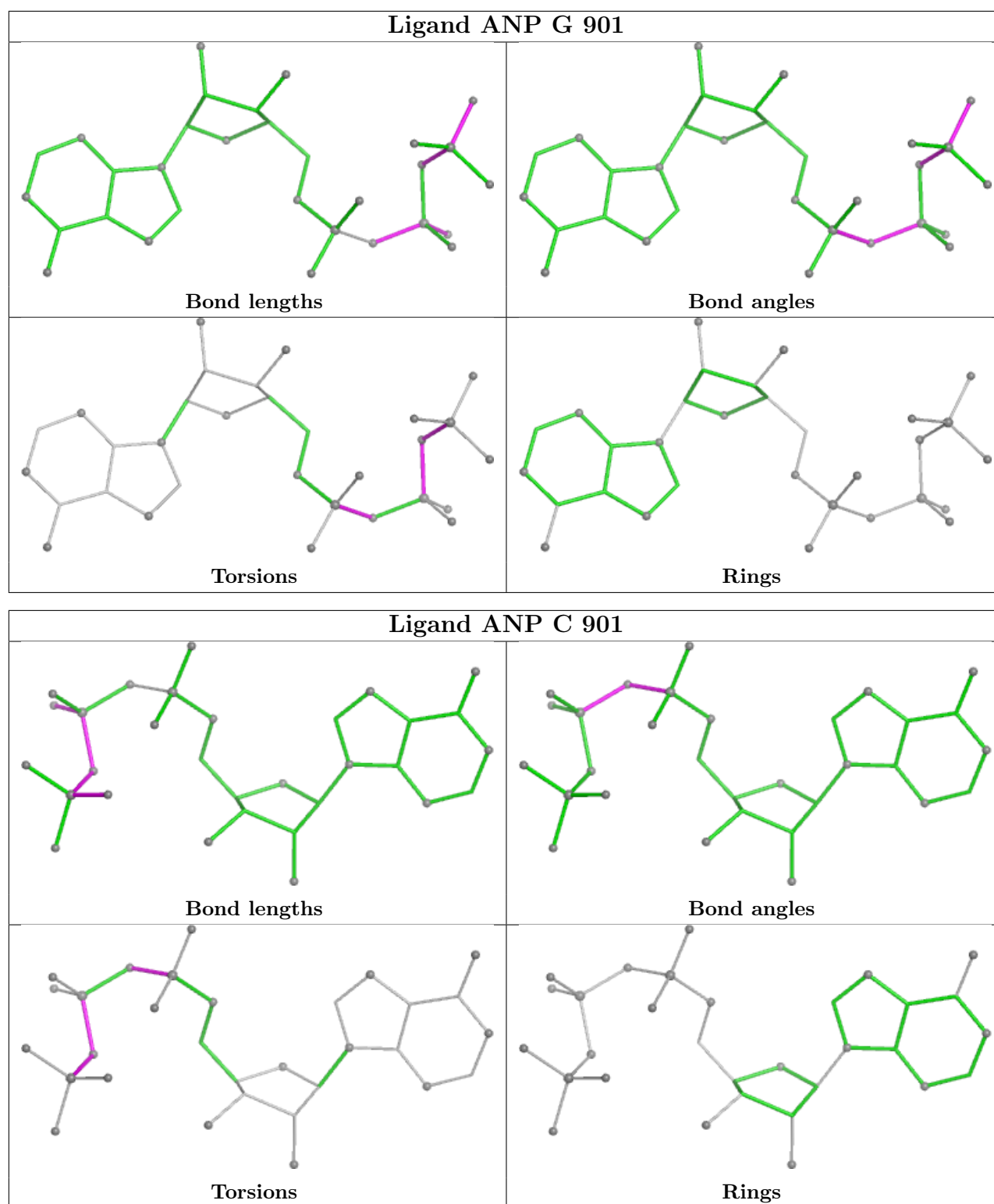
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	262/282 (92%)	-0.36	2 (0%) 82 76	43, 78, 147, 198	0
1	C	261/282 (92%)	-0.20	1 (0%) 88 85	36, 95, 153, 203	1 (0%)
1	F	263/282 (93%)	-0.34	0 100 100	40, 81, 149, 216	2 (0%)
1	G	259/282 (91%)	-0.31	0 100 100	39, 97, 162, 182	1 (0%)
2	A	288/333 (86%)	-0.04	2 (0%) 84 79	75, 118, 165, 250	0
2	D	290/333 (87%)	-0.11	2 (0%) 84 79	41, 108, 171, 247	1 (0%)
2	E	286/333 (85%)	0.04	2 (0%) 84 79	85, 127, 191, 246	0
2	H	284/333 (85%)	-0.20	2 (0%) 84 79	64, 107, 167, 212	0
All	All	2193/2460 (89%)	-0.18	11 (0%) 87 83	36, 105, 171, 250	5 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	253	LEU	3.6
2	H	211	VAL	3.5
2	H	381	LEU	2.7
2	E	381	LEU	2.7
2	A	224	VAL	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

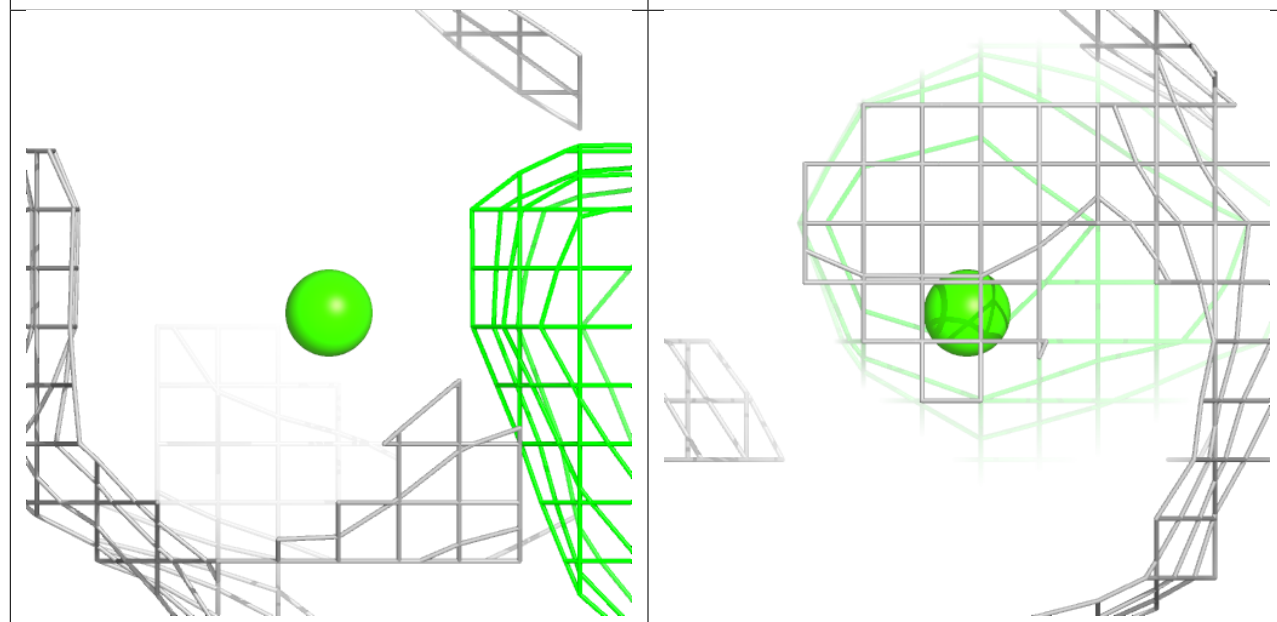
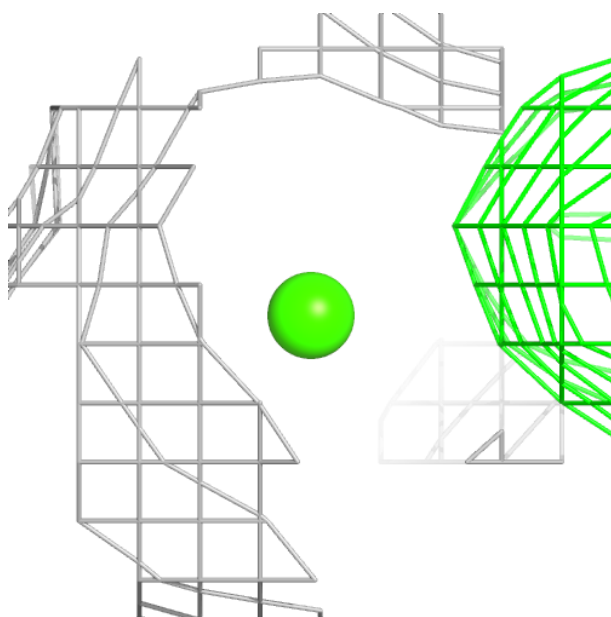
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	D	905	1/1	0.40	0.13	233,233,233,233	0
6	CL	A	903	1/1	0.80	0.16	126,126,126,126	0
3	ANP	B	901	31/31	0.86	0.09	79,114,150,169	0
3	ANP	F	901	31/31	0.86	0.08	81,101,144,157	0
6	CL	D	903	1/1	0.87	0.10	99,99,99,99	0
7	PEG	H	904	7/7	0.88	0.17	100,114,121,126	0
3	ANP	G	901	31/31	0.89	0.09	95,119,156,162	0
3	ANP	H	901	31/31	0.89	0.09	91,113,147,152	0
3	ANP	C	901	31/31	0.89	0.08	87,112,163,165	0
5	GOL	B	903	6/6	0.90	0.18	82,87,104,104	0
7	PEG	D	904	7/7	0.91	0.16	89,94,106,111	0
3	ANP	D	901	31/31	0.92	0.07	98,112,129,139	0
5	GOL	C	903	6/6	0.92	0.17	80,89,93,102	0
3	ANP	A	901	31/31	0.92	0.08	80,101,119,128	0
3	ANP	E	901	31/31	0.93	0.09	70,107,121,122	0
4	CA	H	902	1/1	0.93	0.09	121,121,121,121	0
6	CL	H	903	1/1	0.94	0.09	95,95,95,95	0
4	CA	G	902	1/1	0.94	0.07	125,125,125,125	0
5	GOL	F	903	6/6	0.94	0.12	82,86,90,100	0
4	CA	E	902	1/1	0.96	0.06	104,104,104,104	0
4	CA	D	902	1/1	0.96	0.06	117,117,117,117	0
4	CA	B	902	1/1	0.96	0.04	105,105,105,105	0
4	CA	F	902	1/1	0.98	0.04	110,110,110,110	0
4	CA	C	902	1/1	0.98	0.04	101,101,101,101	0
4	CA	A	902	1/1	0.98	0.04	99,99,99,99	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

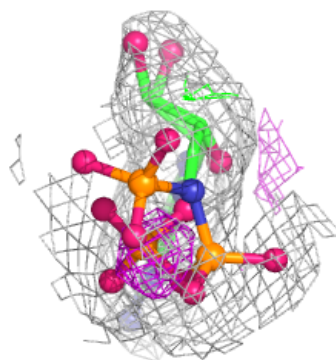
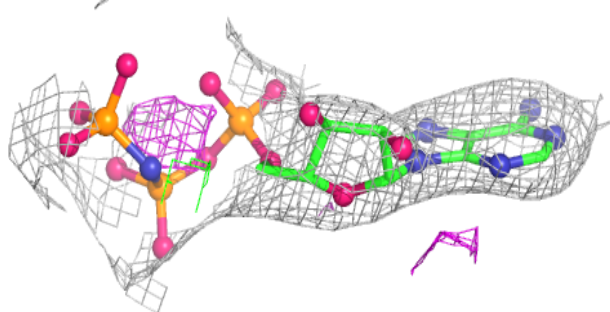
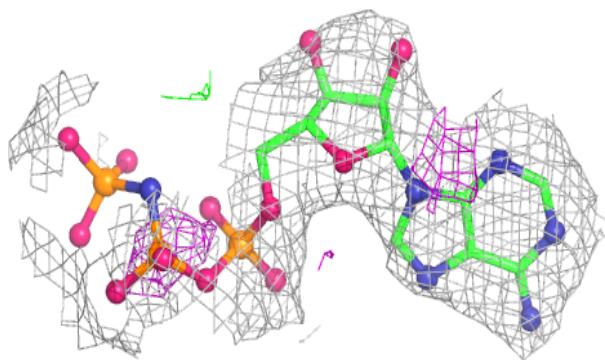
Electron density around CA D 905:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

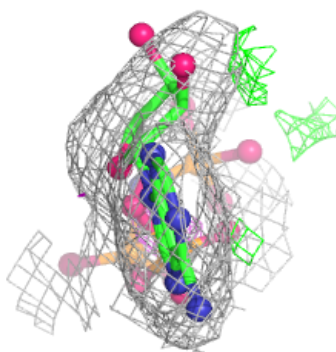
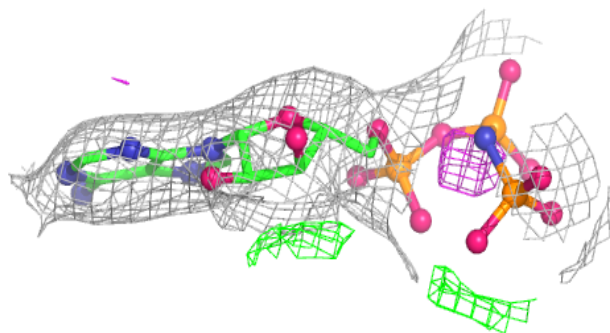
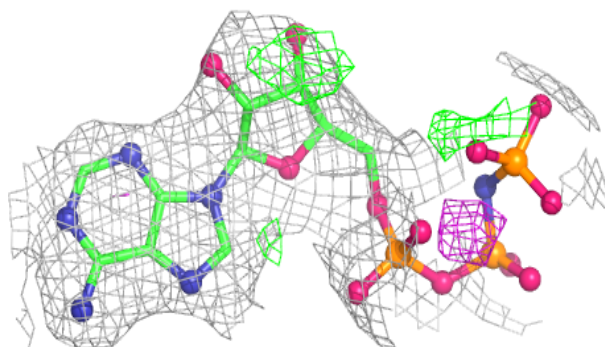


Electron density around ANP B 901:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

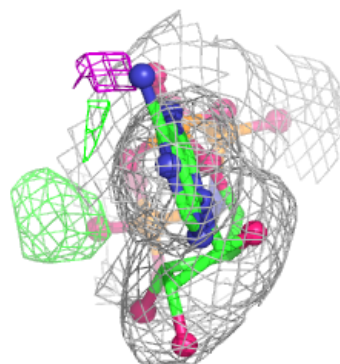
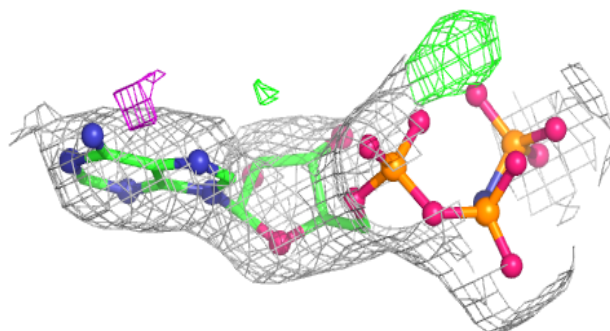
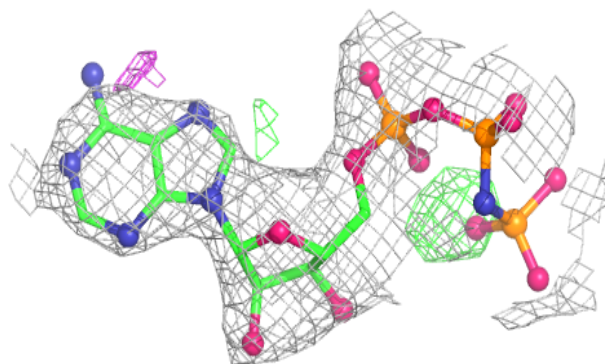
**Electron density around ANP F 901:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

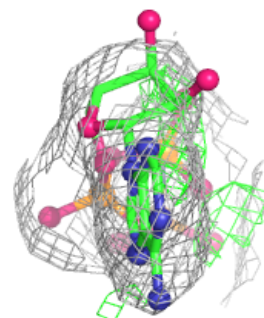
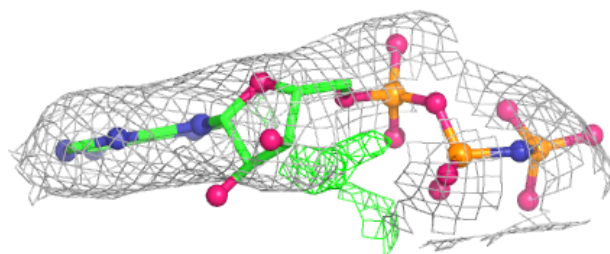
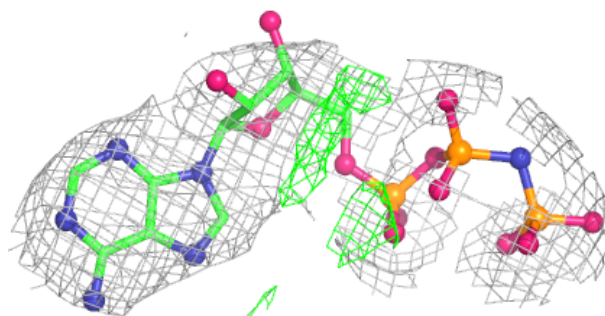


Electron density around ANP G 901:

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and green (positive)

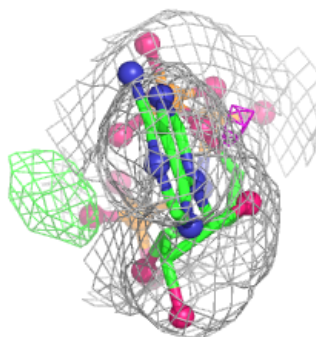
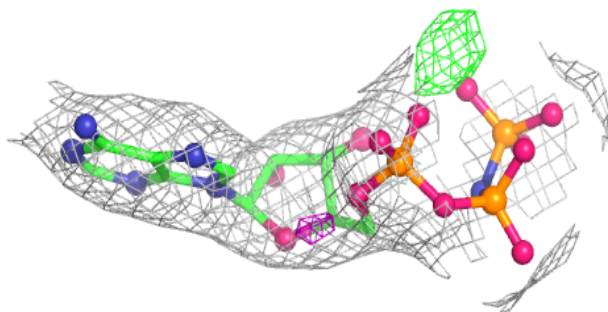
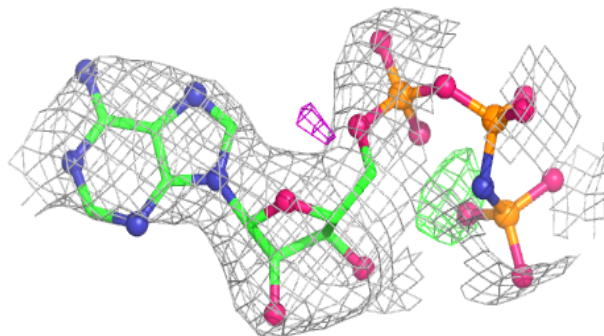
**Electron density around ANP H 901:**

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and green (positive)

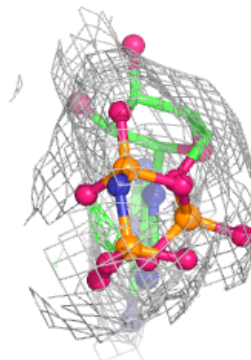
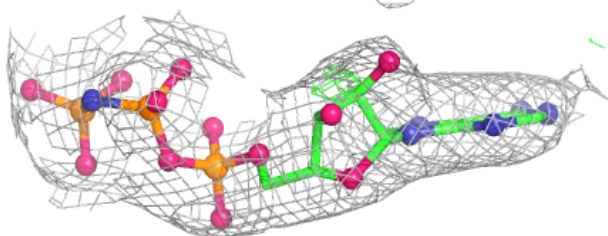
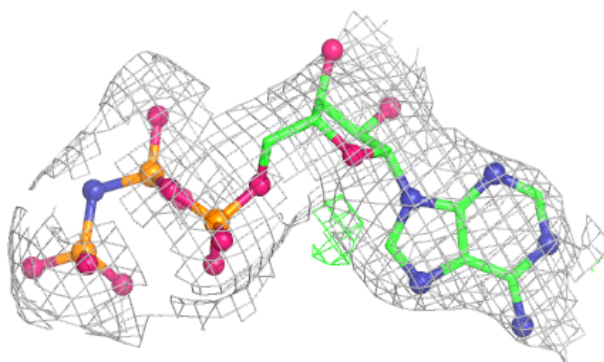


Electron density around ANP C 901:

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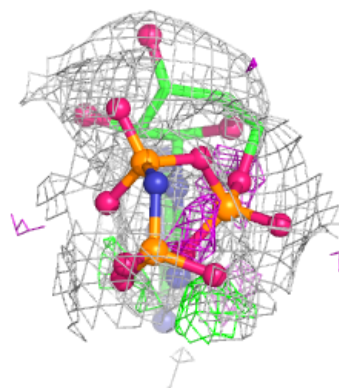
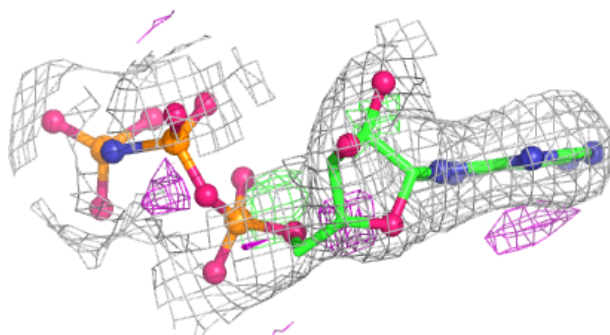
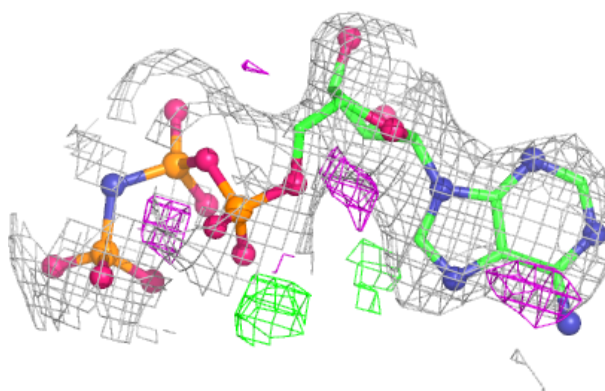
**Electron density around ANP D 901:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

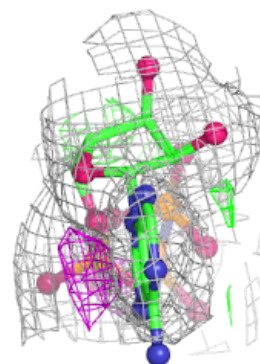
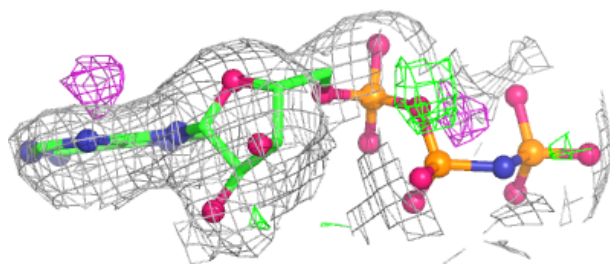
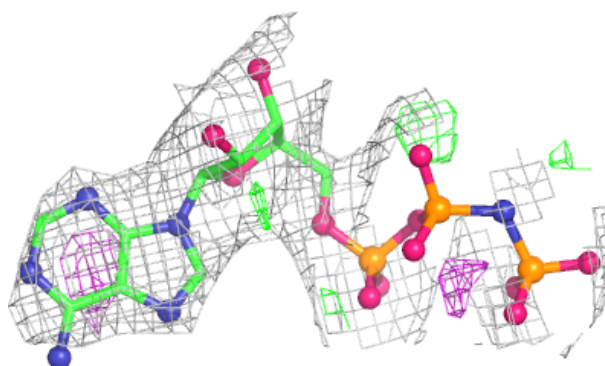


Electron density around ANP A 901:

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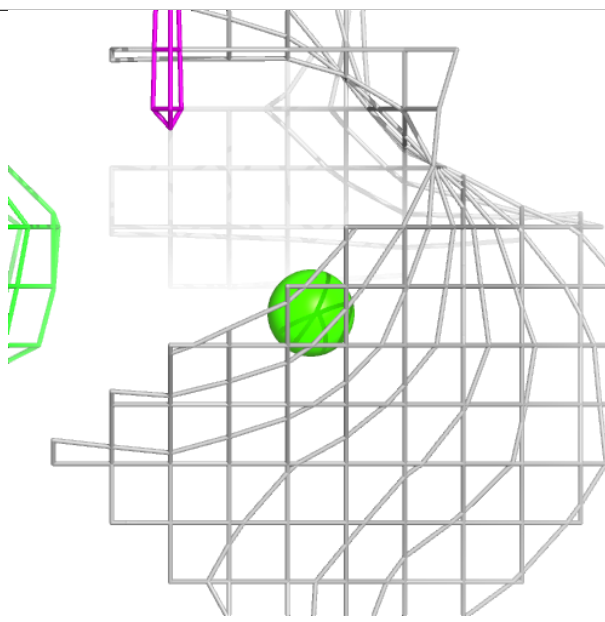
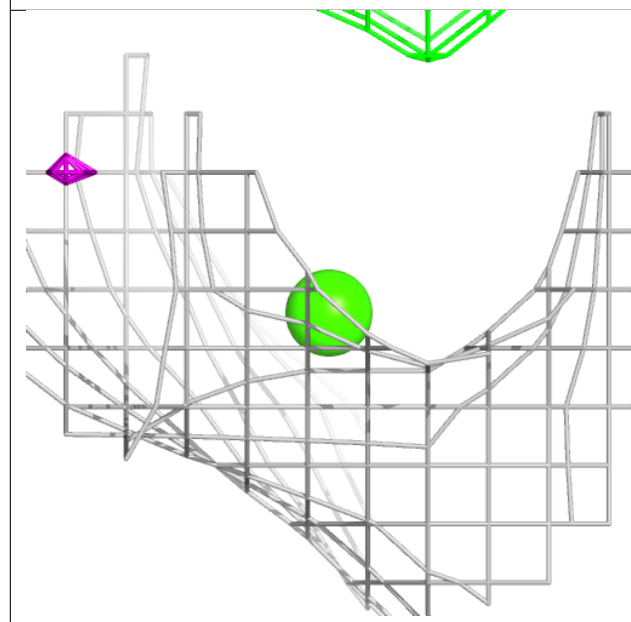
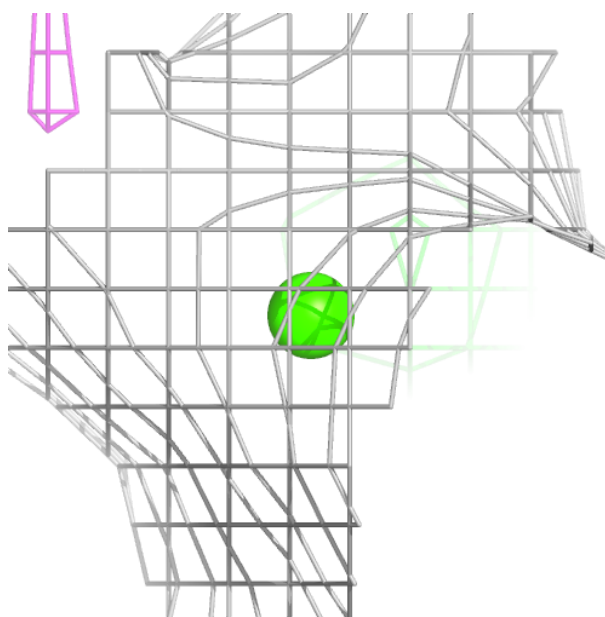
**Electron density around ANP E 901:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



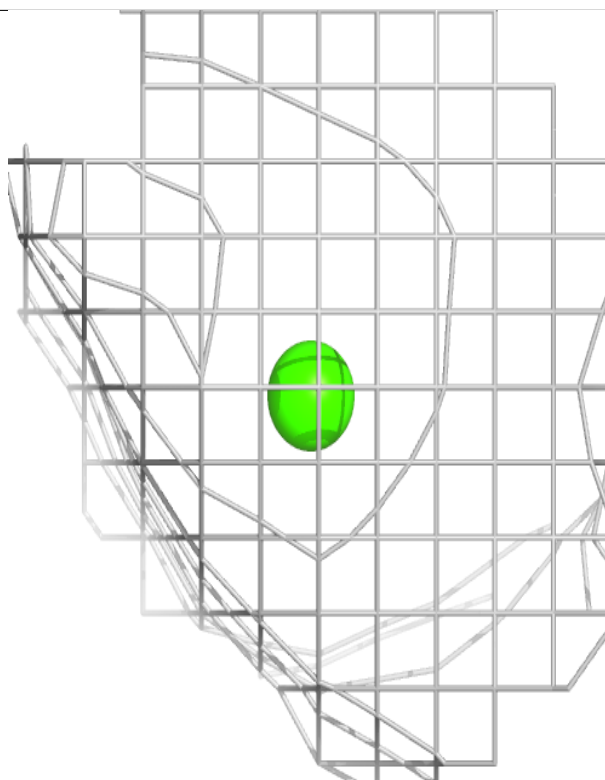
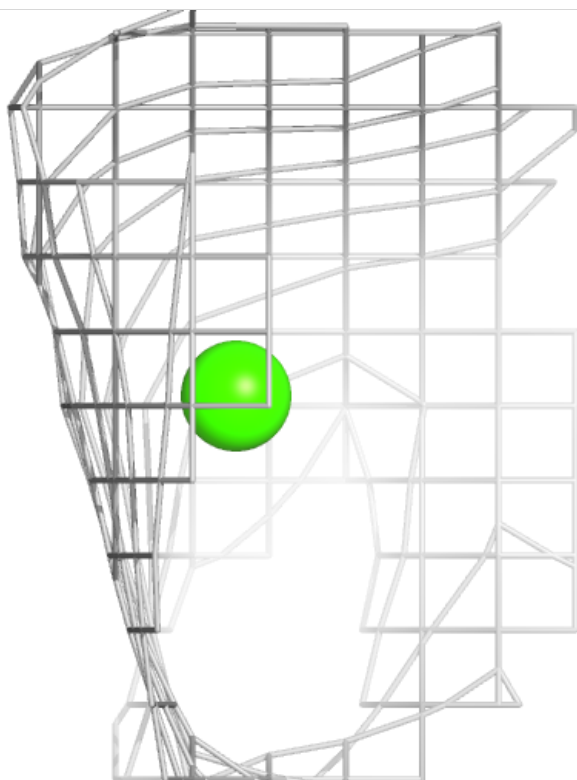
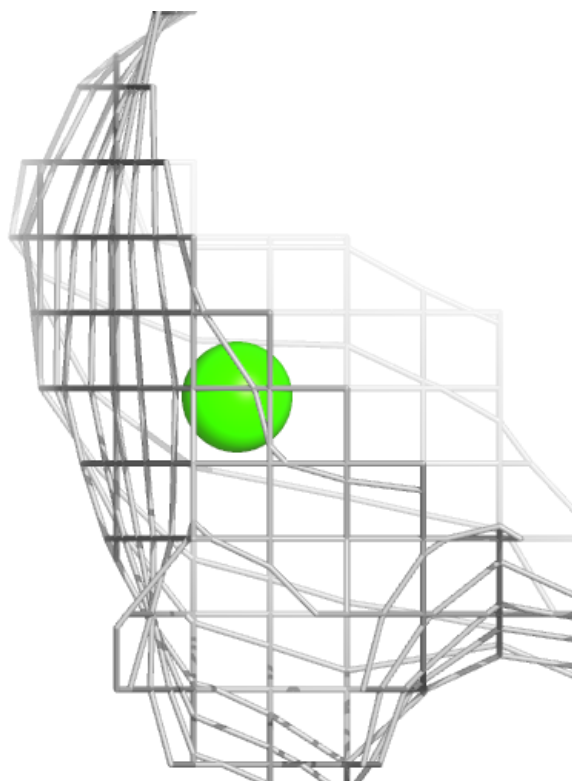
Electron density around CA H 902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



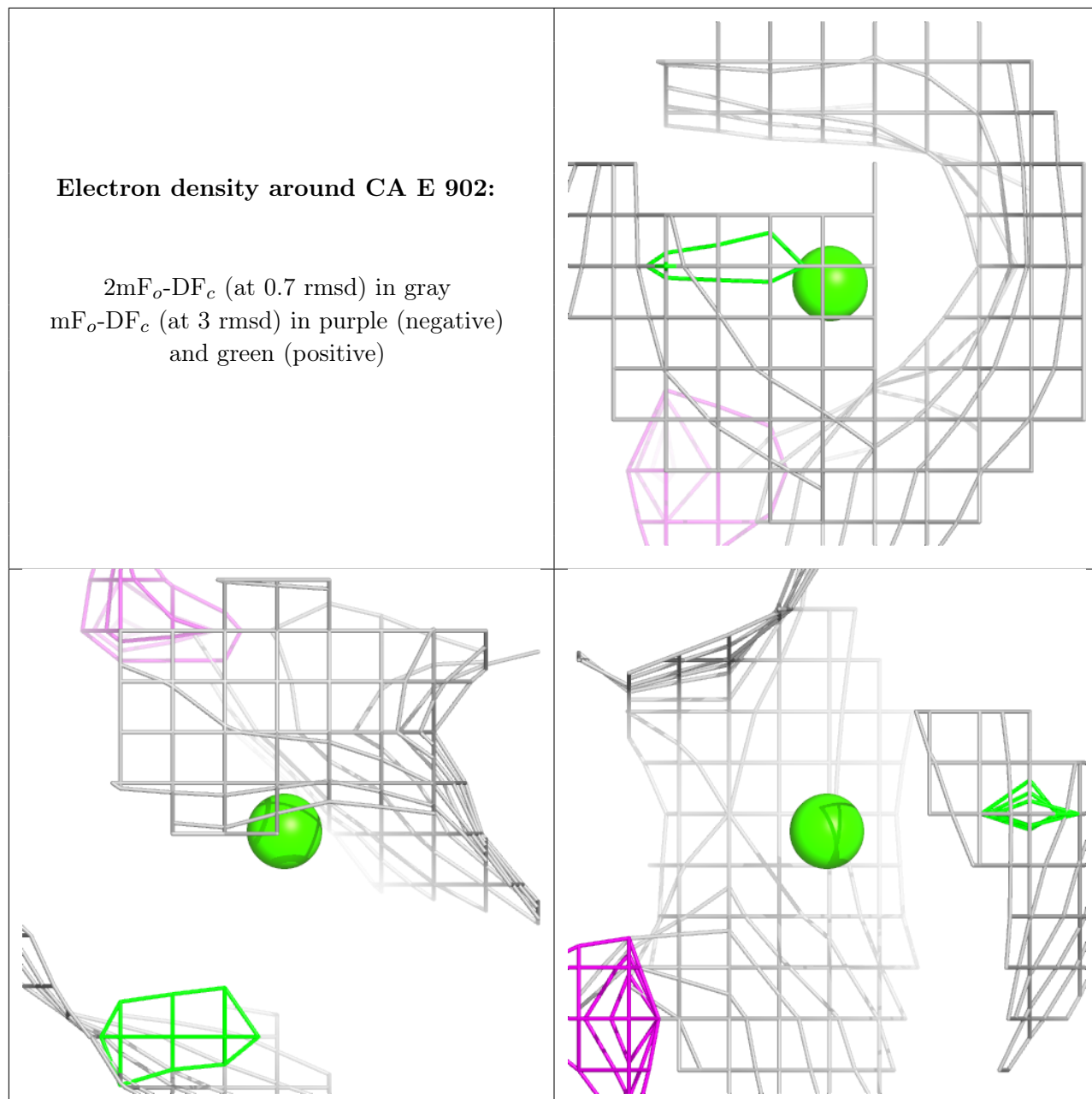
Electron density around CA G 902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



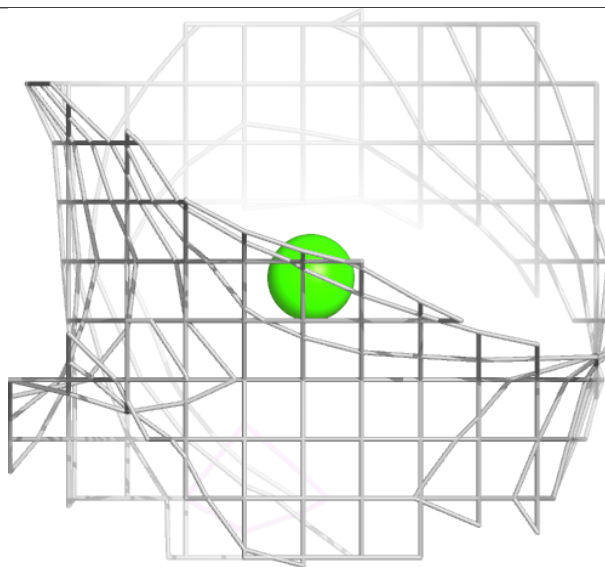
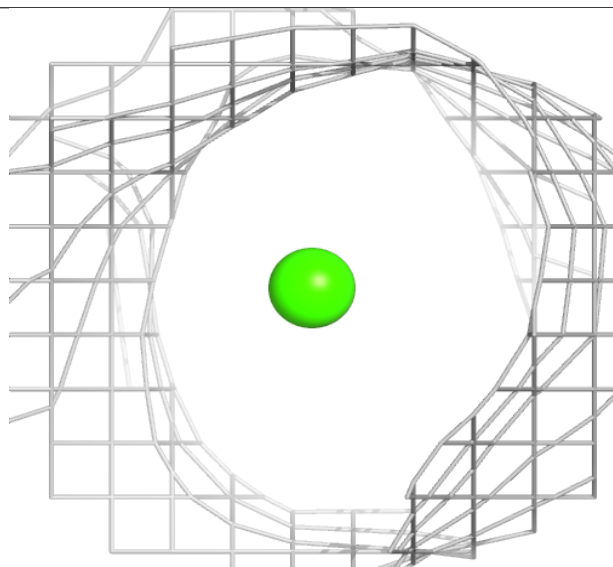
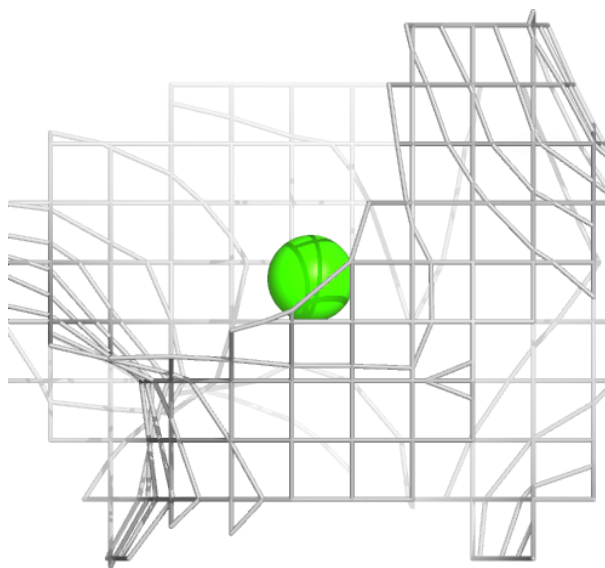
Electron density around CA E 902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



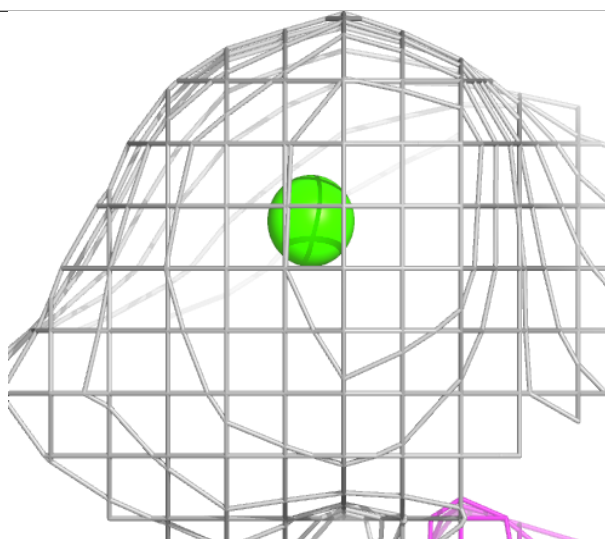
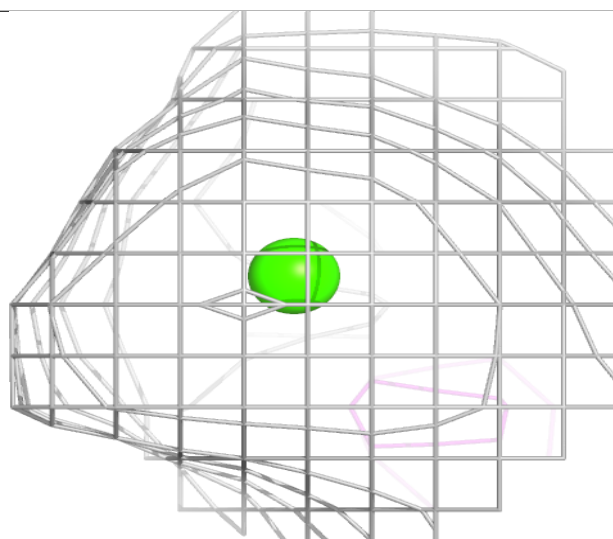
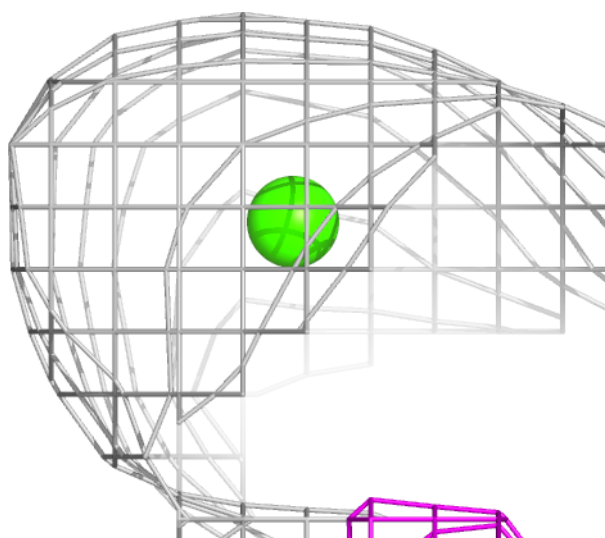
Electron density around CA D 902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



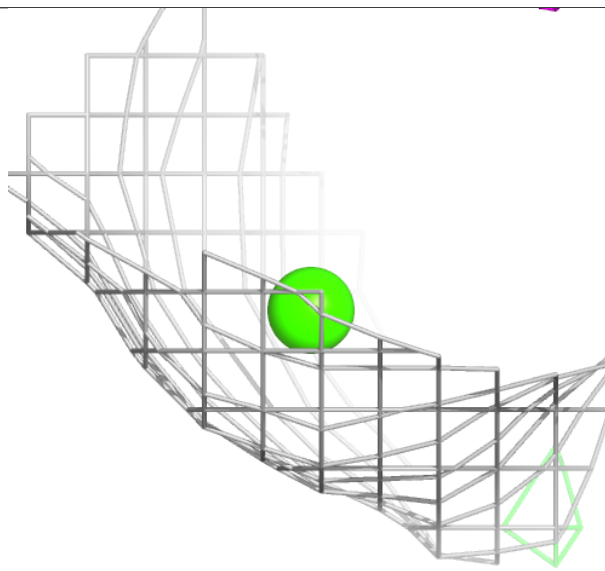
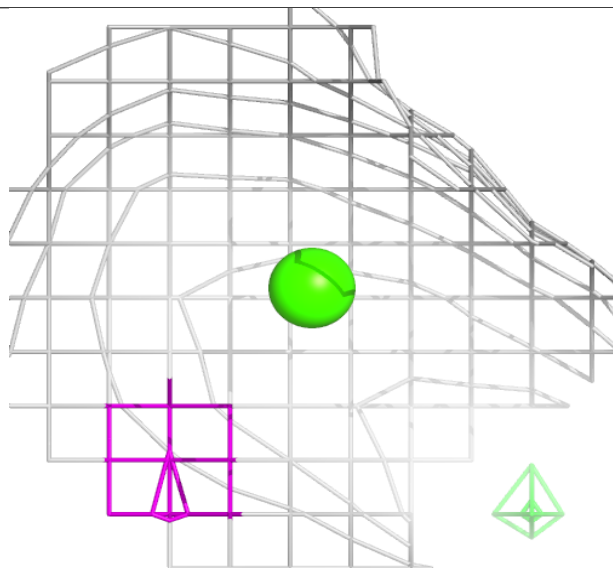
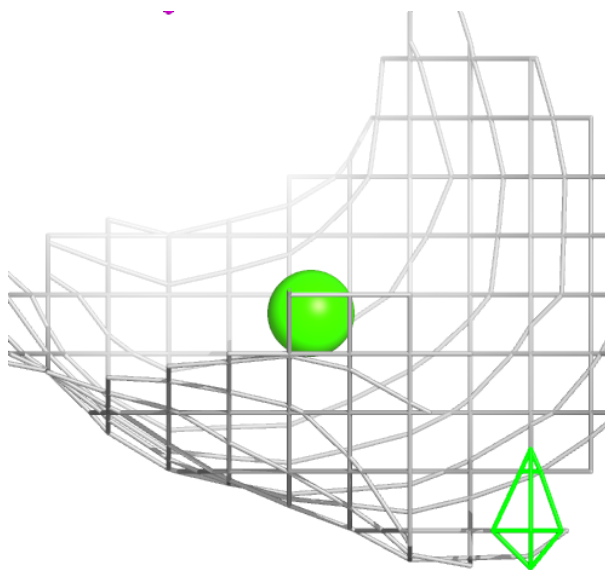
Electron density around CA B 902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



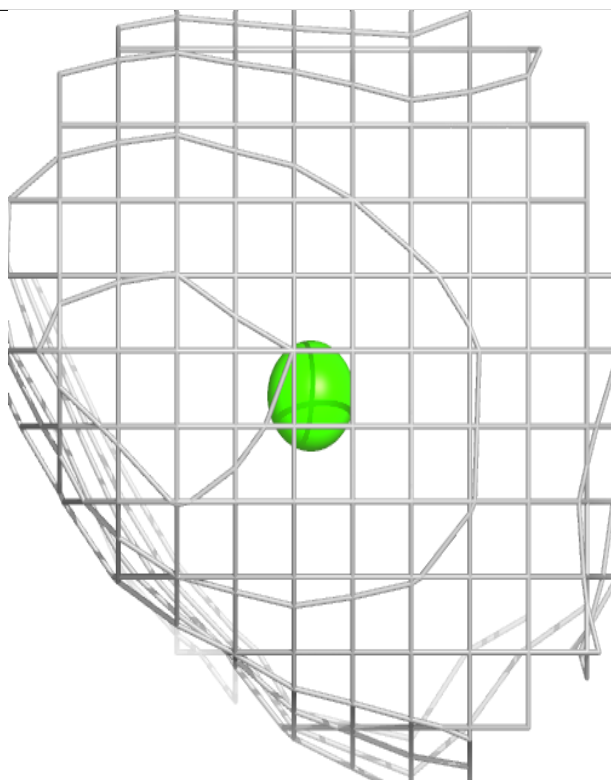
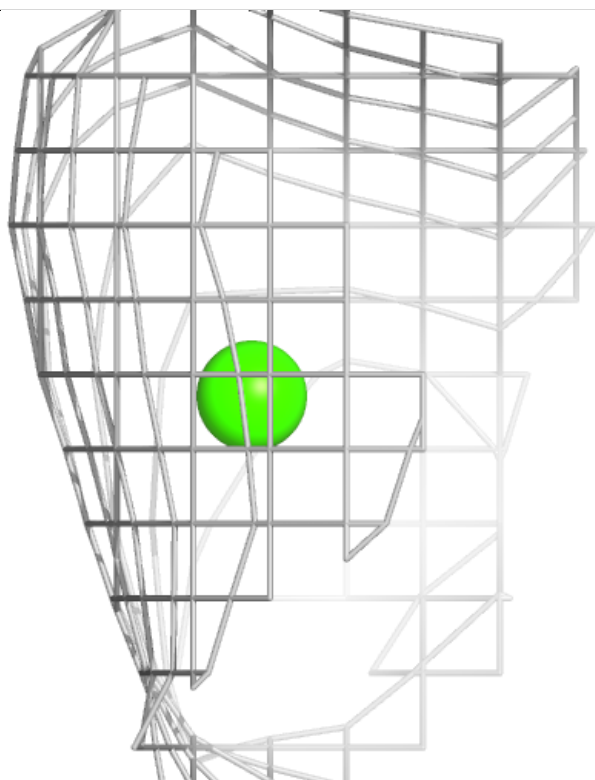
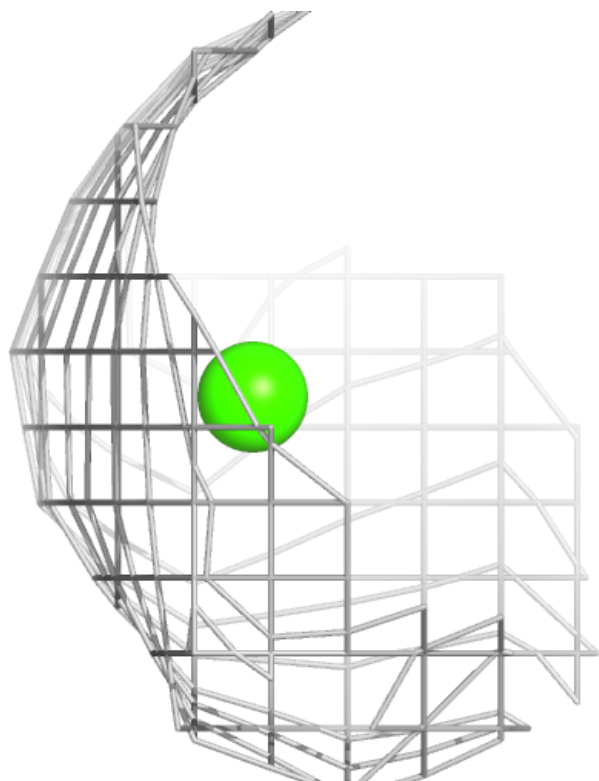
Electron density around CA F 902:

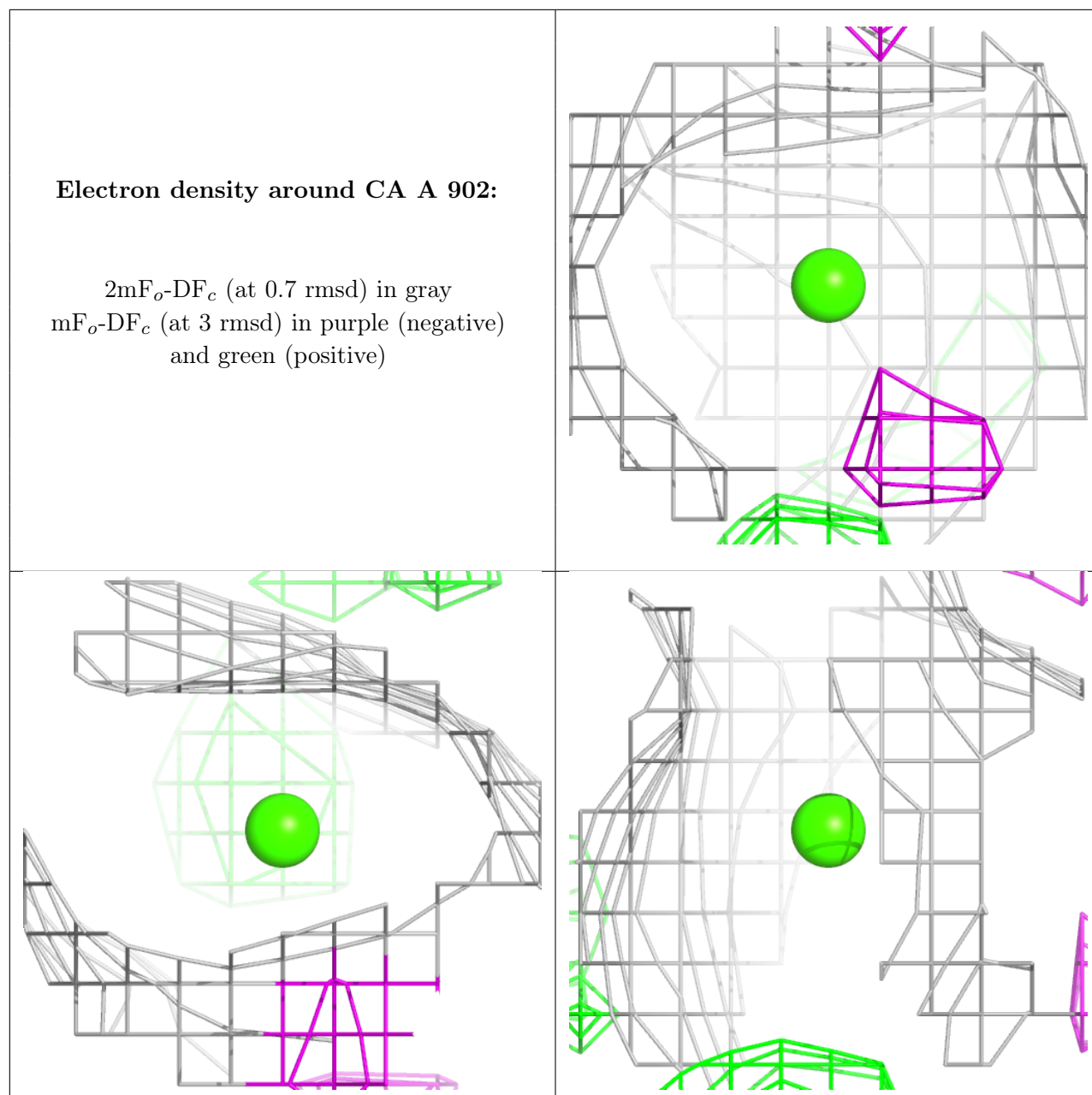
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA C 902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.